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A note on the numerical calculation of asymptotic phases with a numerical study of Hulthén's variational principle

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With 2 figures in the text

An improved method for the calculation of asymptotic phases in quantum mechanical scattering problems is developed. The method is based on the numerical integration of the radial wave equation by using a new modification of Gauss's central difference formula. Applications are made to the computation of some S-phases connected with the Yukawa potential, and a comparison with the results obtained by HULTHÉN according to his variational principle shows that his simplified modification of this principle gives phase values which are extremely accurate even when only a few variational parameters are used.

I. Introduction

The asymptotic phases η_l are of essential importance for the calculation of cross-sections in the quantum mechanical theory of scattering[1], and in the literature various methods have been developed for their computation by means of numerical integration.[1, 2] Since many of these methods are rather laborious to handle practically, we will here give a brief description of a method of numerical integration which is extremely simple and accurate.

II. A modification of Gauss's formulas for numerical integration

The radial wave equation of the scattering problem of a central field is an ordinary differential equation of the second order of the type

$$\frac{d^2 y}{d x^2} = F(x, y) \tag{1}$$

with the initial condition $y = y_0$, $y' = y_0'$ for $x = x_0$. We will use the theory of finite differences for the numerical integration of this equation. Let h be the interval, and let E be the step operator, defined by $Ef(x) = f(x+h)$. Then we will introduce SHEPPARD's central difference operator δ and mean-value operator μ by

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[1] H. FAXÉN—J. HOLTSMARK, Zeits. f. Physik *45*, 307 (1927).

[2] V. ROJANSKY—W. WETZEL, Phys. Rev. *38*, 1979 (1931); P. M. MORSE, Rev. Mod. Phys. *4*, 577 (1932); D. R. HARTREE, R. DE L. KRONIG, and H. PETERSEN, Physica *1*, 895 (1934); R. G. SACHS and M. GOEPPERT-MAYER, Phys. Rev. *53*, 991 (1938); and others.

$$\delta = E^{\frac{1}{2}} - E^{-\frac{1}{2}}, \quad \mu = \frac{1}{2} \cdot (E^{\frac{1}{2}} + E^{-\frac{1}{2}}) \tag{2}$$

with $\mu^2 = 1 + \delta^2/4$, and $\mu(1 + \delta^2/4)^{-\frac{1}{2}} = 1$. Following SHEPPARD[3] we will use operator calculus and symbolic expansions. Taylor's theorem gives immediately $E = \exp(hD)$, where D is the differentiation operator $D = d/dx$. Further we get from eq. (2) that $hD = 2 \sinh^{-1} \delta/2$. The differential equation (1) can therefore be solved by the inverse formula

$$\begin{aligned} h^{-2} y &= \{2 \sinh^{-1} \delta/2\}^{-2} F = \\ &= \delta^{-2} F + \frac{1}{12} F - \frac{1}{240} \delta^2 F + \frac{31}{60\,480} \delta^4 F - \frac{289}{3\,628\,800} \delta^6 F + \cdots, \end{aligned} \tag{3}$$

and the derivative y' can, if required, be obtained from

$$\begin{aligned} h^{-1} y' &= \mu(1 + \delta^2/4)^{-\frac{1}{2}} \{2 \sinh^{-1} \delta/2\}^{-1} F = \\ &= \mu \delta^{-1} F - \frac{1}{12} \mu \delta F + \frac{11}{720} \mu \delta^3 F - \frac{191}{60\,480} \mu \delta^5 F + \frac{2\,497}{3\,628\,800} \mu \delta^7 F - \cdots. \end{aligned} \tag{4}$$

Here the symbols $\delta^{-1} F$ and $\delta^{-2} F$ denote the first and second sums of F, respectively, i.e. $\delta(\delta^{-1} F) = F$ etc. The "integration constants" included in these sums will here be determined by the condition that the formulas under consideration should be valid even in the starting point, $x = x_0$. The equations (3) and (4) were both given by GAUSS, and they have been of fundamental importance for the theory of numerical integration using finite differences.[4] They are here derived only symbolically, but they can also be justified and their remainder-terms can be calculated by using Newton's interpolation formula for unequal intervals with Cauchy's remainder.[5]

Gauss's formula (3) can directly be employed for the calculation of asymptotic phases[6], but here we will instead use a slightly modified form developed by one of us (P.O.L.). The radial wave equation is *linear*, and we will therefore confine ourselves to considering only the simplified form

$$\frac{d^2 y}{dx^2} + g(x) y = f(x). \tag{5}$$

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[3] W. F. SHEPPARD, Proc. London Math. Soc. *31*, 449 (1899). See also J. G. L. MICHEL, J. Inst. Actuar. *72*, 470 (1946); W. G. BICKLEY, J. Math. Physics *27*, 183 (1948).

[4] ENCKE, Berliner Astr. Jahrbuch 1837, ibid. 1867; COWELL, Greenwich Obs. 1909; C. STÖRMER, Videnskapsselskapets skr. Oslo, Mat. natv. kl. 1913, no. 4, 10, and 14; J. JACKSON, Mon. Not. Roy. Astr. Soc. *84*, 602 (1924); D. R. HARTREE, Mem. Proc. Lit. Phil. Soc. Manchester *77*, 91 (1933).

[5] H. P. NIELSEN, Arkiv f. mat. fysik o. astr. *4*, no. 21 (1908); E. J. NYSTRÖM, Acta Soc. Fennicae *50*, no. 13 (1926); J. F. STEFFENSEN, Skan. Aktuarietidskr. *7*, 1 (1924); and others.

[6] See, for instance, R. A. BUCKINGHAM in MOTT and MASSEY, *Theory of Atomic Collisions*, 2nd ed. (Oxford 1949), p. 129.

This special case has also been treated by other authors.[7] Transforming the F-term in eq. (3) to the left member[8], we obtain

$$
\begin{gathered}
y\left\{h^{-2}+\frac{g(x)}{12}\right\}-\frac{1}{12}f(x)=\delta^{-2}F+\gamma, \\
F=-g(x)\cdot y+f(x), \quad \gamma=-\frac{1}{240}\delta^{2}F+\frac{31}{60\,480}\delta^{4}F-+\cdots.
\end{gathered} \tag{6}
$$

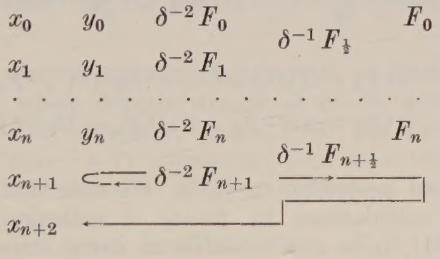
The derivative y' can be found from the relation

$$
h^{-1}y'=\mu\delta^{-1}F-\frac{1}{12}hF'-\frac{1}{3}\mu\delta\gamma+\frac{19}{378}\mu\delta^{3}\gamma-+\cdots \tag{7}
$$

which is easily derived from (4) by using the central difference formula for F' and eq. (6) for the difference correction γ. According to (6) and (7) the initial values of the first and second sums of F are then given by[9]

$$
\begin{gathered}
\delta^{-2}F_{0}=y_{0}\left\{h^{-2}+\frac{g_{0}}{12}\right\}-\frac{1}{12}f_{0}-\gamma_{0}, \\
\delta^{-1}F_{\frac{1}{2}}=\frac{1}{2}F_{0}+h^{-1}y_{0}'+\frac{1}{12}hF_{0}'+\frac{1}{3}\mu\delta\gamma_{0}-\frac{19}{378}\mu\delta^{3}\gamma_{0}+\cdots.
\end{gathered} \tag{8}
$$

Let us now first consider the case when the interval h has been choosen so small that the difference correction γ can be entirely neglected in the whole range of integration. The numerical integration of (5) can then be carried out by using the recurrence rule indicated by the arrow in the scheme below:



$$
\begin{array}{lllll}
x_{0} & y_{0} & \delta^{-2}F_{0} & & F_{0} \\
 & & & \delta^{-1}F_{\frac{1}{2}} & \\
x_{1} & y_{1} & \delta^{-2}F_{1} & & \\
\cdot & \cdot & \cdot & \cdot & \cdot \\
x_{n} & y_{n} & \delta^{-2}F_{n} & & F_{n} \\
 & & & \delta^{-1}F_{n+\frac{1}{2}} & \\
x_{n+1} & \leftarrow & \delta^{-2}F_{n+1} & \longrightarrow & \\
x_{n+2} & \longleftarrow & & &
\end{array} \tag{9}
$$

If the value of y_n has been recorded, it is possible to compute F_n from eq. (6″) and to find $\delta^{-1}F_{n+\frac{1}{2}}$ and $\delta^{-2}F_{n+1}$ by successive summations:

$$
\delta^{-1}F_{n+\frac{1}{2}}=\delta^{-1}F_{n-\frac{1}{2}}+F_{n}, \quad \delta^{-2}F_{n+1}=\delta^{-2}F_{n}+\delta^{-1}F_{n+\frac{1}{2}}. \tag{10}
$$

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[7] W. E. MILNE, Amer. Math. Monthly *49*, 96 (1942); L. FOX and E. T. GOODWIN, Proc. Camb. Phil. Soc. *45*, 373 (1949).

[8] Compare B. NOUMEROV, Publ. Observatoire Astrophys. Cent. Russie, vol. ii, Moscou 1923; Mon. Not. Roy. Astr. Soc. *84*, 592 (1924).

[9] In the following we will use the abbreviations $y_r = y(x_0 + rh)$ etc.

Then y_{n+1} can be obtained according to (6′) by an addition and a division, and the process can be repeated for the next step. If the functions $f(x)$ and $g(x)$ were tabulated in advance, we have found it possible to carry through this process by the aid of only ordinary desk machines with nine figures in the calculation with a rapidity of 60—80 steps an hour.

In comparison to the methods proposed by HARTREE[4], by HARTREE, KRONIG and PETERSEN[2], or by BUCKINGHAM[6], we note that here no Taylor expansion is used in the start and that further no estimations are necessary.

In many problems, in which the integration has to be extended over a wide range demanding an enormous number of steps, this manner of proceeding can be rather laborious. In such cases it seems better to use a larger interval h and to take the difference correction γ into full account. In considering γ it is suitable to divide the integration into three parts: the start, the marching process, and the aftercorrection.

In the start region we will determine the correction γ by using a method of successive approximations. We let an upper index indicate the order of approximation. In a zero-order approximation we put $\gamma^{(0)} = 0$, and some values of $y^{(0)}$ and $F^{(0)}$ around the starting point are then computed according to (6) and (9). From the values of $F^{(0)}$ and its differences a first-order approximation $\gamma^{(1)}$ of the difference correction can be determined, and the start is then repeated until two consecutive series of $\gamma^{(k)}$ agree. In most cases the first approximation appears to have a sufficient degree of accuracy.

When a sufficient number of values of F has been found, we will proceed in another way in order to spare work. Let us assume that the values of y and F up to the point $x = x_0 + nh$ have been computed, and that the corresponding difference scheme of F has been recorded. If ∇ denotes the backward difference operator $\nabla = 1 - E^{-1}$, the quantities in the last backward line n in this scheme may be denoted by $F_n, \nabla F_n, \nabla^2 F_n, \nabla^3 F_n, \ldots$ They may be used for *extrapolating* the difference correction, for from the symbolic relation $E = (1 - \nabla)^{-1} = 1 + \nabla + \nabla^2 + \cdots$ and (2) we easily derive the extrapolation formulas

$$\begin{aligned} \delta^2 F_{n+1} &= \nabla^2 F_n + 2\nabla^3 F_n + 3\nabla^4 F_n + 4\nabla^5 F_n + \cdots, \\ \delta^4 F_{n+1} &= \nabla^4 F_n + 3\nabla^5 F_n + 6\nabla^6 F_n + 10\nabla^7 F_n + \cdots, \end{aligned} \tag{11}$$

and then γ_{n+1} is formed according to (6‴). We note that the elementary series (11) are suitable for calculations by means of ordinary desk machines.[10] By using (6), (10), and (11), it is now possible to carry through the integration in a quite straightforward way, and we will therefore characterize this part of the calculation as a "marching process", which gives a preliminary solution y_{prel}.

Afterwards, when the marching process has been completed for the whole range of integration (including some additional points), it is possible to improve the accuracy of the solution by utilizing the *actual* values of $\delta^2 F_n$, $\delta^4 F_n, \ldots$ found on later stages of the calculation. The final solution is then determined by the formula

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[10] In order to be fit for use the series (11) must be rapidly convergent, which can be obtained by choosing the interval h not too large. However, in general it is convenient to calculate the differences of F only up to the order p where the irregularities, due to the effect of rounding-off errors, become to be of about the same magnitude as the differences themselves; then the formulas (11) correspond to an extrapolation of F and its differences by a polynomial of the degree p.

$$y_{n,\,\mathrm{final}} = y_{n,\,\mathrm{prel}} + h^2 (\gamma_{n,\,\mathrm{actual}} - \gamma_{n,\,\mathrm{extrapolated}}). \tag{12}$$

The idea of the method is that the "aftercorrection" in (12) shall be so small that, in reality, it will be only a check of the extrapolations (11), possibly influencing the last figure in y. The interval h can therefore not be choosen too large.

If the difference correction is taken into full account in this way, we have found it possible to carry out the numerical integration by means of only ordinary desk machines with nine figures in the calculation with a rapidity of 20—30 steps an hour.

Finally, in comparison to the methods proposed by MILNE[7] and by FOX and GOODWIN[7], we note that the solution y is here obtained directly in summed form, which is an advantage; see the discussion by JACKSON.[4]

III. Calculation of eigenfunctions and asymptotic phases

The radial wave equation of the scattering problem connected with the central field $V(r)$ can be written in the form

$$L\Psi \equiv \frac{d^2\Psi}{d r^2} + \left\{k^2 - \frac{l(l+1)}{r^2} + v(r)\right\}\Psi = 0, \tag{13}$$

where $v(r)$ represents the potential and k is the wave number:

$$k^2 = \frac{8\pi^2 m}{h^2} E, \quad v(r) = -\frac{8\pi^2 m}{h^2} V(r). \tag{14}$$

Following HULTHÉN we will assume that $v(r)$ is at least sectionally continuous and bounded in the whole domain except at $r = 0$, where it may be singular as $c_1/x^p - c_2/x^2$, $p < 2$, c_1 arbitrary, and $c_2 \geqq 0$. For the sake of simplicity we will further assume that $r\,v(r)$ approaches zero as r tends to infinity, but we note that the following discussion without difficulties can be generalized to include even the Coulomb case.

The solution with the initial condition $\Psi(0) = 0$, $\Psi'(0) = 1$, has the asymptotic form

$$\Psi(r) \sim A \sin\left(k r - \frac{l\pi}{2} + \eta_l\right), \tag{15}$$

where η_l is the asymptotic phase giving the partial cross-section connected with the l-scattering.

Starting from the initial condition, we can integrate the wave equation (13) numerically be means of the method described in Sec. II. The integration has to be performed up to the point $r = r_1$, where $v(r)$ begins to be negligible in comparison to k^2, and for $r \geqq r_1$ the solution has then the form

$$\Psi(r) = \text{const.}\ \{\sin\eta_l G_2(r) + \cos\eta_l G_1(r)\} \tag{16}$$

with

$$G_1 = \left(\frac{\pi k r}{2}\right)^{\frac{1}{2}} J_{l+\frac{1}{2}}(kr), \quad G_2 = (-1)^l \left(\frac{\pi k r}{2}\right)^{\frac{1}{2}} J_{-l-\frac{1}{2}}(kr), \tag{17}$$

Here $J_p(x)$ are the Bessel functions of the first kind. The asymptotic phase η_l can then be determined from the relation

$$\operatorname{tg}\eta_l = -\left(\frac{\Psi G_1' - \Psi' G_1}{\Psi G_2' - \Psi' G_2}\right)_{r \geq r_1}, \tag{18}$$

where the derivative Ψ' may be computed from (4) or from the linear algebraic equation (7). A good check on the calculations is obtained by computing the constant η_l for different values of r.

In order to investigate the propagation of errors in our integration scheme (9), we have also considered another way of integration. Following MILNE[11] we put $\Psi = \omega \sin\chi$ with the auxiliary condition $\chi' = \alpha\,\omega^{-2}$, $\alpha =$ arbitrary constant, which for ω gives the equation

$$\frac{d^2\omega}{dr^2} + \left\{k^2 - \frac{l(l+1)}{r^2} + v(r)\right\}\omega - \frac{\alpha^2}{\omega^3} = 0, \tag{19}$$

which again can be numerically integrated by the Gaussian formula (3). This equation has previously been used for investigating the asymptotic behaviour by ROJANSKY and WETZEL[2], by MORSE[2], by HARTREE, KRONIG and PETERSEN[2], and by ARNOT.[12] We have integrated eq. (19) *inwards*, starting from the initial condition $\omega(\infty) = (\alpha/k)^{\frac{1}{2}}$, $\omega'(\infty) = 0$. We have then connected the solution ω with the wave function Ψ, found by starting from $r = 0$, in an arbitrary point $r = r_c$ by the formula

$$\frac{\Psi'}{\Psi} = \frac{\omega'}{\omega} + \frac{\alpha}{\omega^2}\cot\chi. \tag{20}$$

The asymptotic phase η_l can then be found from the relation

$$\eta_l - \frac{\pi l}{2} = \operatorname{arccot}\left\{\frac{\omega^2}{\alpha}\left(\frac{\Psi'}{\Psi} - \frac{\omega'}{\omega}\right)\right\}_{r=r_c} - k r_c + \alpha\int_{r_c}^{\infty}\left(\omega^{-2} - \frac{k}{\alpha}\right) dr. \tag{21}$$

The formulas (20) and (21) were first given by HARTREE, KRONIG, and PETERSEN.[2] We note that the result must be independent of r_c and of the value of α; for the sake of simplicity we have choosen $\alpha = k$. We have compared the different values of η_l obtained according to (18) or to (21) in some typical cases, see Table I, and, since the agreement was excellent, we have concluded that the propagation of error in the scheme (9) could be entirely neglected. For values of k, which are not too large, we have therefore found it convenient to use formula (18) alone. It is, of course, much simpler to integrate the linear equation (13) by means of (6) than to integrate the non-linear equation (19) by using (3).

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[11] W. E. MILNE, Phys. Rev. *35*, 863 (1930); H. A. WILSON, Phys. Rev. *35*, 948 (1930); E. L. HILL, Phys. Rev. *38*, 1258 (1931); L. A. YOUNG, Phys. Rev. *38*, 1612 (1931). E. MADELUNG, Zeits. f. Physik *67*, 516 (1931) has treated the special case $\alpha = 1$.

[12] F. L. ARNOT, Proc. Camb. Phil. Soc. *32*, 161 (1936).

IV. Applications to the Yukawa potential (S-phases). Comparison with the results obtained according to Hulthén's variational principle

According to HULTHÉN[13] and others[14, 15, 16], the asymptotic phases or the solution of the scattering problem can be determined from a variational principle by using a series of approximate wave functions $\Psi_1, \Psi_2, \Psi_3 \ldots$ with an increasing number of parameters c_ν. HULTHÉN considered the integral

$$L = \int_0^\infty \Psi L \Psi \, d r, \tag{22}$$

for all functions Ψ having the boundary conditions

$$\Psi(0) = 0, \quad \Psi(r) \sim \sin\left(k r - \frac{l \pi}{2} + \eta\right) \tag{23}$$

with different phases η. Varying the function Ψ around the exact solution Ψ, HULTHÉN obtained the formula

$$\delta L + k \delta \eta = 0. \tag{24}$$

If Ψ is varied in such a way that the additional condition $L = 0$ is always fulfilled ($\delta L = 0$), this gives $\delta \eta = 0$, which means that the asymptotic phase has a *stationary* character. Since, in general, the "eigenphase" is not an extremum, the variational principle must in this case be treated with special caution, and HULTHÉN has worked out two criterions for the accuracy of the results obtained.

HULTHÉN's original formulation of the variational principle was rather complicated in the applications, since the equations for $\operatorname{tg}\eta$ or $\cot\eta$ appeared to be of the second degree. Recently he has therefore developed a new modification[17] of his method for calculating S-phases, which is considerably simpler. The new method consists of two steps, of which the first is again based on a variational principle. By dropping the condition $L = 0$, HULTHÉN obtains now *linear* equations for the parameters c_ν. The first step gives only preliminary values η' and L' for the phase and the integral (22), respectively, but the phase value can be essentially improved in the second step. Putting $\delta\eta = \eta' - \eta''$ and $\delta L = L' - L'' = L'$ into formula (24), we get immediately the relation

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[13] L. HULTHÉN, K. Fysiogr. Sällsk. Lund Förhandl. *14*, no. 21 (1944); ibid. *14*, no. 8 (1944); C. R. X$^{\text{me}}$ Congrès des Math. Scan. 1946, Copenhagen 1947, p. 201; compare also Arkiv f. mat., fysik o. astr. *29* B, no. 1 (1942).

[14] E. A. HYLLERAAS, Fra Fysikkens Verden (NIELS BOHR issue), Oslo 1945; A. PAIS, Proc. Camb. Phil. Soc. *42*, 45 (1946); N. ZEILON, K. Fysiogr. Sällsk. Lund Förhandl., N. F. *58*, no. 10 (1947); I. E. TAMM, J. Exp. Theor. Phys. *18*, 337 (1948); ibid. *19*, 74 (1949).

[15] W. KOHN, Phys. Rev. *74*, 1763 (1948); S. S. HUANG, Phys. Rev. *76*, 477 (1949); ibid. *76*, 867 (1949).

[16] J. SCHWINGER, Phys. Rev. *72*, 742 (1947); "Lectures on Nuclear Physics", Harvard University 1947; J. M. BLATT—J. D. JACKSON, Phys. Rev. *76*, 18 (1949); B. A. LIPPMANN—J. SCHWINGER, ibid. *79*, 469 (1950); B. A. LIPPMANN, ibid. *79*, 481 (1950).

[17] L. HULTHÉN, Arkiv f. mat., fysik o. astr. *35* a, no. 25 (1948).

$$\eta'' = \eta' + \frac{1}{k} L' \tag{25}$$

where η'' is the improved phase value.[18]

In this modified form of HULTHÉN's variational principle with its two steps, it is not so easy to get an analytical test of the accuracy of the final result for the asymptotic phase, even if HULTHÉN's two criterions give a rough estimation of the accuracy of the wave functions. In such a case, it may therefore be of some interest to study the final accuracy in some typical results by means of numerical methods.

In order to carry out a comparison with HULTHÉN's results[17], we have treated eq. (13) with the Yukawa potential $v(r) = 1.5\, e^{-r}/r$, belonging to the deuteron problem, for $l = 0$ and for $k = 0.1, 0.2, \ldots, 1.0$. The numerical integration was carried out according to Sec. II with eight or nine figures in the calculation and the intervals $h = 0.1$ and $h = 0.2$. By using ordinary desk machines (Facit ESA), it was possible for us to record a wave function for a given k-value and to find the corresponding phases within 8—9 hours, including the start and the check of the integration. The results are contained in Tables I—III and in Figs. 1 and 2.

Table I

A study of the numerical accuracy and of the propagation of errors in the integration scheme (9), obtained by using outward and inward solutions connected in the point $r = r_c$; see formula (21)

$$v(r) = 1.5\, e^{-r}/r,\; l = 0,\; k = 0.2,\; I = k \int_{r_c}^{\infty} (\omega^{-2} - 1)\, dr$$

r_c	cot $(\chi_c - kr_c)$	I	cot η
6	0.671 1752	0.000 1511	0.670 9561
8	0.670 9801	165	0.670 9562
10	0.670 9590	19	0.670 9563
12	0.670 9566	2	0.670 9563
14	0.670 9563	0	0.670 9563

Table II contains a comparison between HULTHÉN's phases[17] and the values computed by us. It is perhaps somewhat surprising that so extremely good phase values can be obtained by using HULTHÉN's modified principle when

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[18] It may be noted that, by putting $\eta' = 0$, $\Psi = G_1$ into (25), one gets the well known formula for η in BORN's approximation.

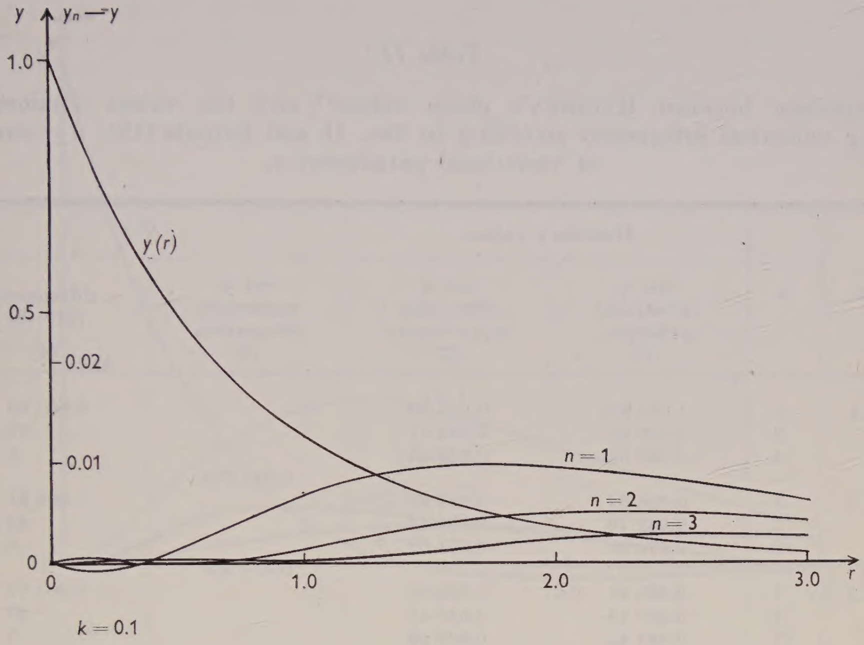

Fig. 1.

only one, two, or three variational parameters are used. We note that the first-order improvement (25) is essential for this result.

Finally we have investigated how HULTHÉN's approximate wave functions tend against the accurate function obtained by numerical integration. HULTHÉN's functions are of the form

$$\begin{aligned} \Psi_n(r) &= \sin(kr + \eta) - y_n(r) \cdot \sin \eta, \\ y_n(r) &= e^{-r} + (1 - e^{-r}) \sum_{\nu=1}^{n} c_\nu e^{-\nu x}, \end{aligned} \tag{26}$$

where $y_n(r)$ gives the deviation from the "asymptotic" form in the neighbourhood of $r = 0$. Figures 1 and 2 contain for $k = 0.1$ and $k = 1.0$, respectively, the function $y(r)$ found from the numerically calculated wave function $\Psi(r)$ by a normalization to the amplitude $A = 1$ for large values of r. In another scale the same figures contain also the differences $y_n(r) - y(r)$ for $n = 1, 2, 3$, i.e. the errors in HULTHÉN's approximations. It appears that HULTHÉN's functions $y_n(r)$ give good approximations of $y(r)$, and that the convergency is almost uniform in the whole range for r. A good wave function $\Psi(r)$ can therefore be obtained by using (26), the constants c_ν found from the variational principle in the first step, and the phase value η found from (25) in the second step.

Table II

Comparison between HULTHÉN's phase values[17] and the values obtained by using numerical integration according to Sec. II and formula (18). n = number of variational parameters c_ν

k	n	Hulthén's values			
		cot η variational principle (1)	cot η first-order improvement (2)	cot η numerical integration (3)	difference (2) − (3) (4)
0.1	1	1.021 92	0.984 50		0.000 90
	2	0.999 36	0.983 67		27
	3	0.990 84	0.983 46		6
	—			0.983 395	
0.2	1	0.698 03	0.671 87		0.000 91
	2	0.682 49	0.671 19		23
	3	0.676 55	0.671 02		6
	—			0.670 956	
0.3	1	0.665 21	0.639 57		0.001 01
	2	0.650 14	0.638 81		25
	3*	0.644 45	0.638 63		7
	—			0.638 563	
0.4	1	0.698 73	0.670 87		0.001 12
	2	0.682 42	0.669 99		24
	3*	0.676 30	0.669 82		7
	—			0.669 753	
0.5	1	0.754 17	0.722 74		0.001 15
	2	0.735 96	0.721 80		21
	3*	0.729 15	0.721 64		5
	—			0.721 594	
0.6	1	0.817 52	0.781 52		0.001 06
	2	0.796 89	0.780 60		14
	3	0.789 19	0.780 47		1
	—			0.780 455	
0.7	1	0.883 73	0.842 04		0.000 87
	2	0.860 21	0.841 25		8
	3	0.850 89	0.841 17		0
	—			0.841 171	
0.8	1	0.950 99	0.902 21		0.000 58
	2	0.924 19	0.901 65		2
	3	0.914 18	0.901 63		0
	—			0.901 629	
0.9	1	1.019 14	0.961 20		0.000 24
	2	0.990 12	0.960 96		0
	3*	0.973 53	0.960 99		3
	—			0.960 961	
1.0	1	1.089 28	1.018 71		−0.000 14
	2	0.992 61	1.018 97		+12
	3	1.033 87	1.018 92		7
	—			1.018 854	

* Private communication from Prof. L. Hulthén.

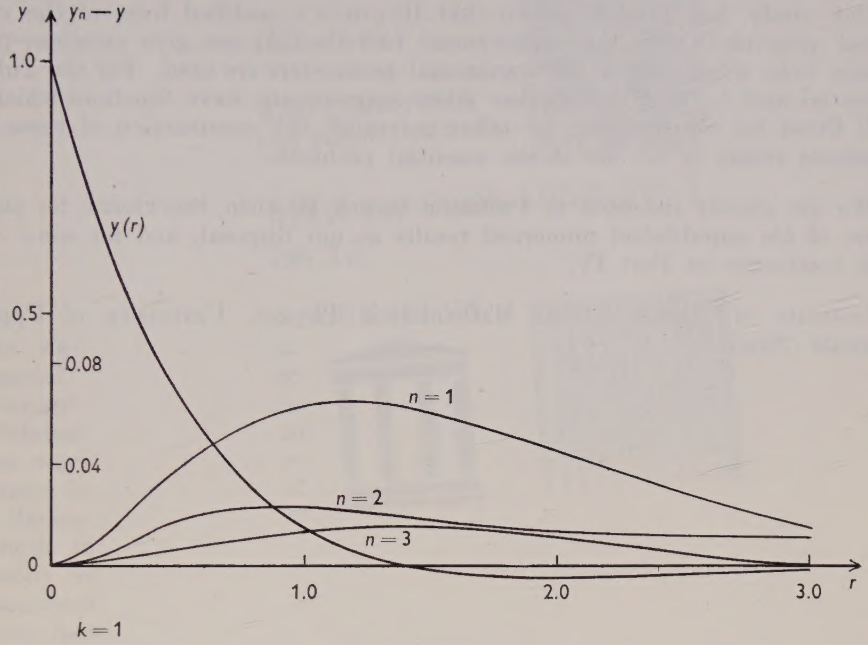

Fig. 2.

A comparison between Table III, which contains HULTHÉN's criterion ratios ϱ_1 and ϱ_2, and Figs. 1 and 2 shows that the quantities $|\varrho_1 - 1|$ and $|\varrho_2 - 1|$ can roughly be taken as measures of the errors $y_n - y$.

Table III

HULTHÉN's criterion ratios ϱ_1 and ϱ_2 for $k = 0.1$ and $k = 1.0$. These quantities are equal to 1 for the exact solution. n = the number of variational parameters

	$k = 0.1$		$k = 1.0$	
n	$\varrho_1 - 1$	$\varrho_2 - 1$	$\varrho_1 - 1$	$\varrho_2 - 1$
1	−0.00 55	−0.00 89	−0.04 26	−0.00 64
2	−0.00 23	+0.00 48	+0.01 59	+0.01 54
3	−0.00 11	−0.00 29	−0.00 90	+0.00 34

V. Comments

We have found that, by means of the methods developed in Secs. II and III, it is possible to calculate a wave function and the corresponding asymptotic phase with an accuracy of 3—4 figures within a few hours and with an accuracy of 6—7 figures within 8—9 hours by using only ordinary desk machines.

Our study has further shown that HULTHÉN's modified form of the variational principle[17] with the improvement formula (25) can give excellent phase values even when only a few variational parameters are used. For the Yukawa potential and $l = 0$, HULTHÉN has given approximate wave functions which are well fitted for the purpose; for other potentials the construction of these trial functions seems to be one of the essential problems.

We are greatly indebted to Professor Lamek Hulthén, Stockholm, for placing some of his unpublished numerical results at our disposal, and for some valuable comments on Part IV.

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